DEVICE MODELING

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This is the summary report of the activities of the device modeling workshop which was held as a part of the Space Photovoltaic Research and Technology Conference at the Lewis Research Center, October 7-9, 1986. A partial list of the participants in the workshop is attached as Appendix A.

The purpose of this workshop was to access the status of solar cell device modeling to see if it is meeting the present and future needs of the Photovoltaic Community working on the development of space solar cells.

During the course of this workshop the following questions were addressed:

- 1. How are present models being used?
- 2. What models are now available?
- 3. Why does one use finite difference, finite element or Monte Carlo methods? What problems are associated with each of these techniques?
- 4. Is the existing database adequate?
- 5. What additional experimental work is needed?
- 6. What additional theoretical work is needed?
- 7. How do you model superlattice devices?
- 8. Should dial-up access to detailed numerical models be provided?
- 9. Can or should detailed models be applied to radiation damaged studies?

Model Uses

Solar cell models find application throughout the cell development cycle. They are used as a design guide both for determining the factors limiting present performance of solar cells as well as providing comparison between competing solar cell designs. Models are used for performance prediction for cells which have not yet been built, operating under conditions for which they have not been tested. An example of this is the comparison of vertical junction cells, etched junction cells, conventional cells, and IBC cells, from one sun to a thousand suns, carried out for

Sandia using two dimensional silicon models. Models find extensive use in the analysis of experimental data. The more detailed and complex numerical models are frequently used to verify simpler analytic models to establish their validity and to establish the conditions under which the simplier models give valid results.

Types of Models

Analytic

In general analytic models are those for which sufficient simplifying assumptions have been applied such that closed form solutions to the equations can be found. These types of models have the advantage that they require relatively little computing time. The existence of closed form solutions allows for easy intuitive examination of the application of a model. The disadvantage is that, in many cases, the many approximations needed to reduce the complexity to the point where analytic solutions apply, has over simplified the problem to the point where significant effects have been ignored.

Numerical

Detailed numerical solutions require far fewer approximations, and hence, can deal with many physical effects simultaneously. This means that many of the interactions which occur in a solar cell can be modeled in some detail. One can expect to get excellent agreement between the model and experiments. Numerical models allow for a much more detailed physical description. On the other hand, they are usually far more complex than the analytic models, and as consequence, are less intuitive and certainly much more compute intensive.

Numerical Techniques

Finite Difference

Finite difference techniques are among the simplest way to numerically solve a set of simultaneous differential equations. However, they are, for all practical purposes, restricted to the treatment of solar cells which can be described by rectangular geometries. They are capable of computing current-voltage curves under light and dark conditions, spectral response, and can deal with a variety of spectra, under all conditions from low light intensity to one thousand sun conditions. They

provide a means of examining, in extreme detail, all of the operating mechanisms that are known to influence solar cell performance. The solutions are performed contact to contact. That is, they describe the entire operation of the solar cell without having to segment it into regions.

Finite Element

Finite element techniques are capable of handling non-rectangular geometries and would be useful for describing solar cells such as the V groove or polka dot cells. The finite element technique is one that is frequently employed in stress analysis. It is somewhat more complex than the finite difference technique, but, is capable of all the computations that a finite difference technique can handle.

Monte Carlo

The Monte Carlo formulation involves describing the operation of a solar cell at the particle level. It amounts to tracking the projectory of individual electrons and holes. It's a technique which can be employed to describe the operation of a device when hot carriers are present such as might occur when abrupt hetero structures are employed in the device design or when feature size becomes so small that classical drift and diffusion equations no longer provide an adequate description. The Monte Carlo technique is extremely compute intensive, and in general, requires very fast, very large computers or very long computer run times or perhaps both. additional difficulty is that it involves twice the number of dimensions that either the finite difference or finite element techniques require, since one must use both real space and reciprocal space in the calculations. The technique is also not an efficient method of computing current flow through a PN junction. (It may be possible to find ways to circumvent this problem.) The Monte Carlo technique is applied only in those cases where other more conventional approaches break down. It is unlikely to be used for full contact-to-contact calculations or for the computation of currentvoltage curves and spectral response as are finite difference or finite element technique.

What Are The Modeling Needs Of The Photovoltaic Community?

Two Dimensional (Three Dimensional)

There are a number of conditions under which two (or three) dimensional analysis are required. Cells which have non planar geometry such as a V groove, vertical junction, or point contact cells will require at least two dimensional and perhaps three dimensional models for an adequate description of their performance. Even conventional cells require two dimensional models when operated under high concentration.

Time Dependent Models

Time dependent models, that is those which are capable of modeling transient response, are useful for the analysis of some diagnostic experiments applied to solar cells in which a light or bias conditions are pulsed.

Other Materials

In addition to silicon and GaAs, other materials are being considerd for future application for space cells. These include a wide range of III-V materials as well as thin film materials such as amorphous silicon and CuInSe₂. The physics of operation of the thin film materials is significantly different from that of bulk silicon and GaAs single crystal materials. Models appropriate to thin film devices should be developed. Such models would serve as a useful aid in the design of these devices as well as in the selection of competing device designs and materials.

Database

Considerable discussion occurred as to the adequacy of the materials parameters database. Materials which were considered were silicon, III-V semiconductors, amorphous silicon-germanium and CuInSe₂. For the most part, an adequate database exists for silicon, and, with some noteable exceptions, for the III-V materials being considered for space applications. A possible exception is the data pertaining to InP. In the case of the amorphous silicon materials and thin film CuInSe₂, it was felt that the existing database should have considerable improvement. Among the materials parameters of interest are: the absorption coefficient, as a function of wave length,

composition, and doping; the bandgap is a function of composition and doping; the mobility is a function of composition and doping; and the recombination parameters. In the case of recombination centers, it's imperative to have information about density, energy level, and capture cross sections as a function of position, doping and radiation conditions. For Auger recombination, the auger coefficients need to be known. It was pointed out that a single parameter such as the surface recombination velocity is probably not adequate for very good device modeling, the surface recombination is a function of operating conditions and fabrication procedures.

Device Modeling Under Radiation Damage Conditions

Considerable insight and improvement in radiation hard solar cell designs should result from very careful detailed numerical modeling of solar cell operation in the presence of radiation damage. Some concern was expressed about whether or not enough information was known about the defect structure. Can the defects be characterized adequately with regard to energy levels, capture cross sections, and spatial distribution to be used in numerical codes? The existence of a model which could adequately handle radiation damage would be useful in the analysis of radiation damage experimental data, as well as in the design of radiation hard solar cells.

Superlattice Models

The modeling of superlattices as used in solar cells is in the very early stages. A great deal more work will need to be done before these models are useful in the design or analysis of solar cells.

Dial-Up Availability

It was felt that easy access to a detailed numerical code would be very useful, both for the solar design community, and for people tempting to verify the validity of simplier analytical models. However, some concern was expressed about having someone use these codes who was not expert in their use. Improper specification of input can lead to erroneous output.

Appendix A

Name

Company

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Executive Summary

A workshop on solar cell modeling was held at the Space Photovoltaic Research and Technology Conference on October 7, 1986. The conclusions of this workshop were as follows:

- 1. Solar cell models are a vital tool in the development of more efficient reliable and radiation hard solar cells, they find application throughout the entire cell development cycle.
- 2. While the silicon solar cell models are well developed for both one and two dimensional requirements, there is a need for further development of models which will handle non-rectangular geometries, such as those found in V groove cells and point contact cells.
- 3. Applications involving concentrator cells and new cell designs, such as the point contact cell, will require two and even three dimensional modeling for the efficient design of these cells.
- 4. The prospects for using new materials, such as InP and amorphous silicon for space applications, requires that existing models be extended to these materials. Since physics of operation of thin film amorphous cells is significantly different from that of single crystal cells, extensive model development will be required.
- 5. An opportunity exists in the design of radiation hard solar cells and in the prediction of their degradation due to radiation damage for the coupling of known radiation damage mechanisms with existing detailed numerical models. It is expected that development of radiation damage models using detailed numerical code would allow for comparison of competing designs and accurate prediction of the degraded properties of radiation damaged cells.
- 6. Modeling of superlattice solar cells is in the very early stages and will require considerable work before these models can be used reliably for solar cell design.